Supporting Materials

Synthesis of Palm Sheath Derived-Porous Carbon for Selective CO_2 Adsorption

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1. Breakthrough experiment

The breakthrough experiments were conducted in a homemade apparatus, as shown in Figure S1. The feeding streams are gas-mixtures of 15/85 (v/v) CO_2/N_2 and 10/90 (v/v) CO_2/CH_4 at 298 K and 1.01 bar. In the separation experiment, samples (PSK-2-650, 0.2970 g，13.3 cm) were packed into Φ 4×100 mm stainless steel column, and the column was activated under reduced pressure at 393 K for 24 h. A carrier gas (He ⩾ 99.999%) was used to purge the adsorption bed for about 8 h at room temperature. The gas flows were regulated by a mass flow meter, and the effluent gas stream from the column is monitored by Mass spectrometry (Hidden, UK). After each separation test, the sample was activated by flushing the adsorption bed with helium gas for 2 h at 373 K.

The separation efficiency for binary mixtures in the PS-derived carbons can be simplified and compared in terms of adsorption selectivity, S, defined for binary mixtures as, were calculated according to the IAST model proposed by Myers *et al*.[S1,S2] Where q_1 and q_2 are the absolute component loadings of the adsorbed phase in the mixture at partial pressures P_1 and P_2.

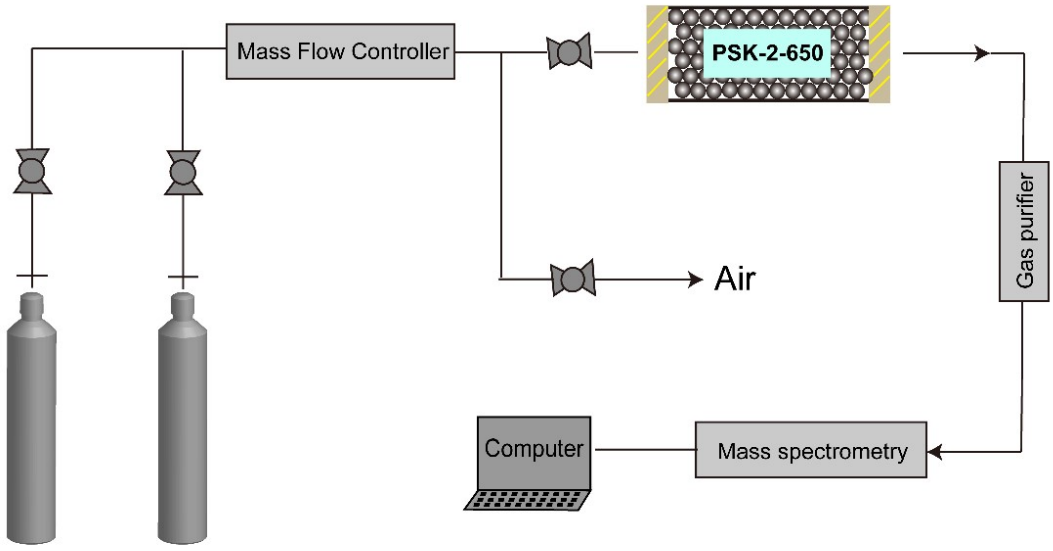

Figure S1. Breakthrough experiments apparatus.

Table S1 Chemical composition determined by elemental analysis and XPS.

carbon	Element analysis (wt%)			XPS (atom%)					
	C	N	O	C	N	O	O-I	O-II	O-III
PS-C	78.95	0.90	12.00	88.33	1.1	10.57	\	\	\
PSK-1-550	72.19	0.43	24.71	82.81	1.11	16.08	36.6	33.4	30.0
PSK-2-650	58.97	0.56	37.41	82.67	1.28	16.04	36.3	33.0	30.7
PSK-3-750	62.84	0.87	33.71	83.32	0.95	15.73	36.1	33.0	30.9

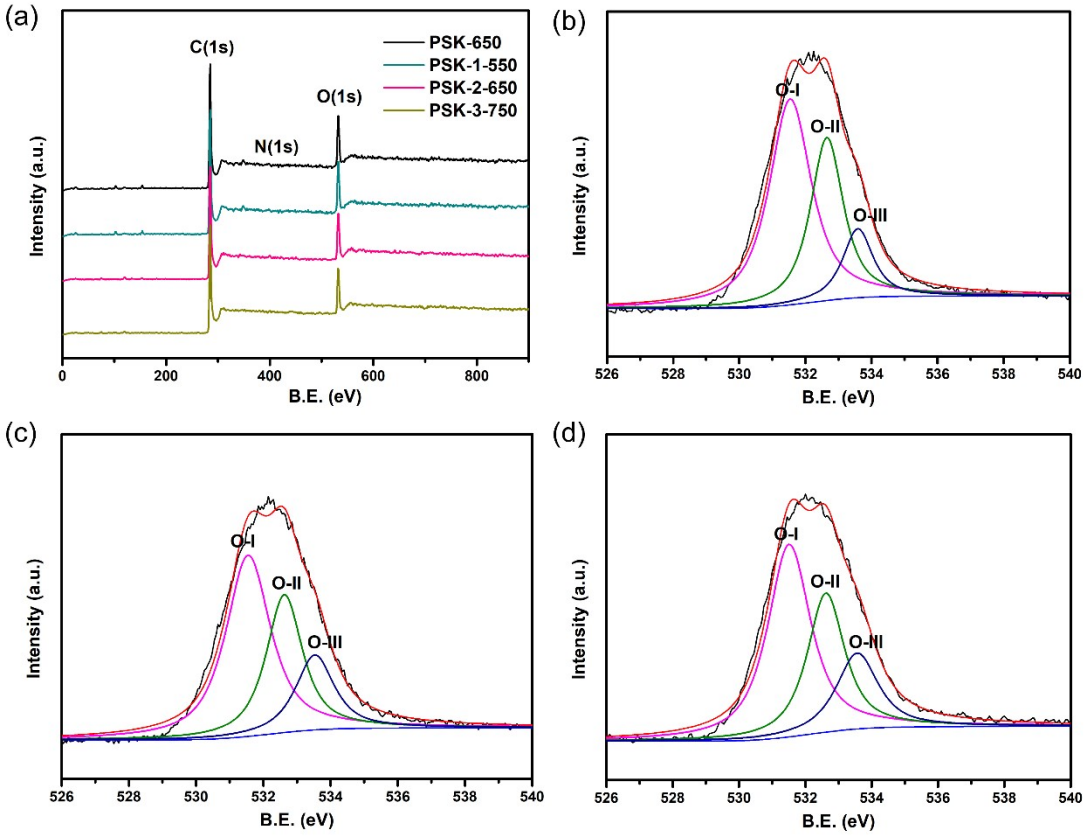

Figure S2. (a) Wide-scan survey XPS spectra of PS-derived carbons; High-resolution O1s signals of (b) PSK-1-550, (c) PSK-2-650, (d) PSK-3-750.

Elemental analysis and X-ray photoelectron spectroscopy (XPS) was used to investigate the elemental compositions of raw palm sheath and the activated carbons (Table S1). From the XPS wide survey spectra, two obvious chemical characteristics of C (284.8 eV) and O (532.8 eV) were observed on PS-derived carbons. After KOH activation, the C and O peaks still exist and there is no visible N peak. The resolution of O1s signal is mainly composed of C=O groups (O-I, 531.5 eV), C-OH/C-O-C groups (O-II, 532.7 eV), and HO-C=O groups (O-III, 533.6 eV), respectively. And the

three components are stable under the variation of activation conditions (Figure S2). We summarized the quantitative analysis results of N and O species in Table S1. The surface N content determined by XPS after activation is 0.95 to 1.10 atom%, which is negligible. Based on the elemental analysis, the PS carbon precursor contains 0.9 wt.%. Despite KOH/PS ratio and activation temperature, the overall nitrogen contents are still low (0.40-0.87wt.%). Due to the negligible nitrogen content in porous carbon, investigating the effect of pore size on gas adsorption and separation performance become possible.

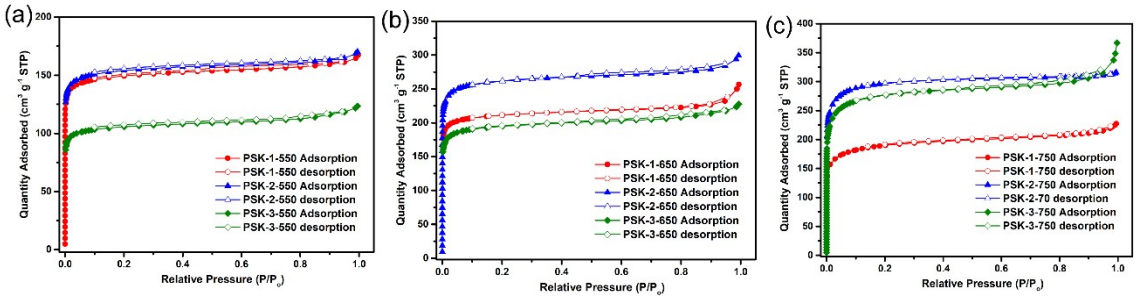

Figure S3. N_2 isotherms of (a) PSK-1-550, (b) PSK-2-650, (c) PSK-3-750.

Table S2 Pore textural properties and CO_2 uptakes of palm sheath-derived carbons at different conditions.

Sample	S_{BET} [a] ($m^2\ g^{-1}$)	Vp [b] ($cm^3\ g^{-1}$)	CO_2 uptake (mmol g^{-1})				CH_4 uptake (mmol g^{-1})	
			273 K 1 bar	298 K 1 bar	273 K 0.15 bar	298 K 0.15 bar	273 K 1 bar	298 K 1 bar
PSK-1-550	480	0.30	3.35	2.70	1.63	1.02	1.62	1.02
PSK-2-550	486	0.26	3.15	2.13	1.40	0.74	1.25	0.89
PSK -3-550	340	0.19	2.59	1.82	1.24	0.71	0.97	0.68
PSK -1-650	671	0.40	4.22	3.07	1.75	1.00	1.87	1.30
PSK -2-650	840	0.46	5.28	3.48	2.00	1.09	2.20	1.47

PSK -3-650	620	0.35	3.80	2.69	1.50	0.86	1.51	1.02
PSK -1-750	715	0.34	4.30	2.86	1.49	0.84	1.87	1.27
PSK -2-750	1052	0.48	4.09	2.60	1.31	0.70	1.72	1.14
PSK -3-750	894	0.54	4.11	2.21	1.14	0.55	1.47	0.98

[a] The specific surface area was determined by the BET equation (P/P_0 = 0.05−0.3). [b] Total pore volume at P/P_0 = 0.99. [c] The micropore volume was estimated as d < 2 nm using the equilibrium model for slit pores. [d] percentage of the volume of micropores in the total pore volume.

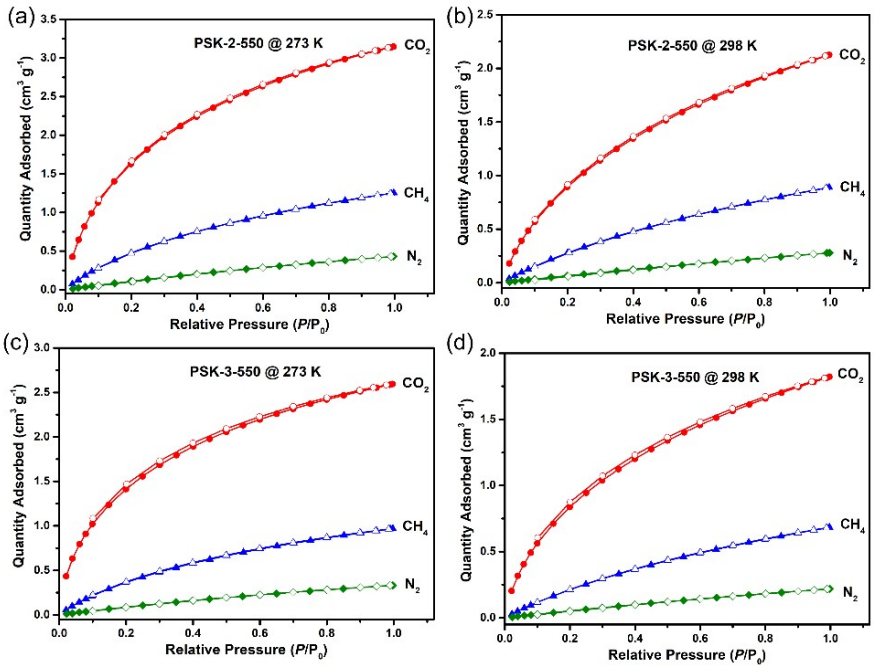

Figure S4. CO_2, CH_4 and N_2 adsorption-desorption isotherms of PS-derived carbons activated at 550 °C

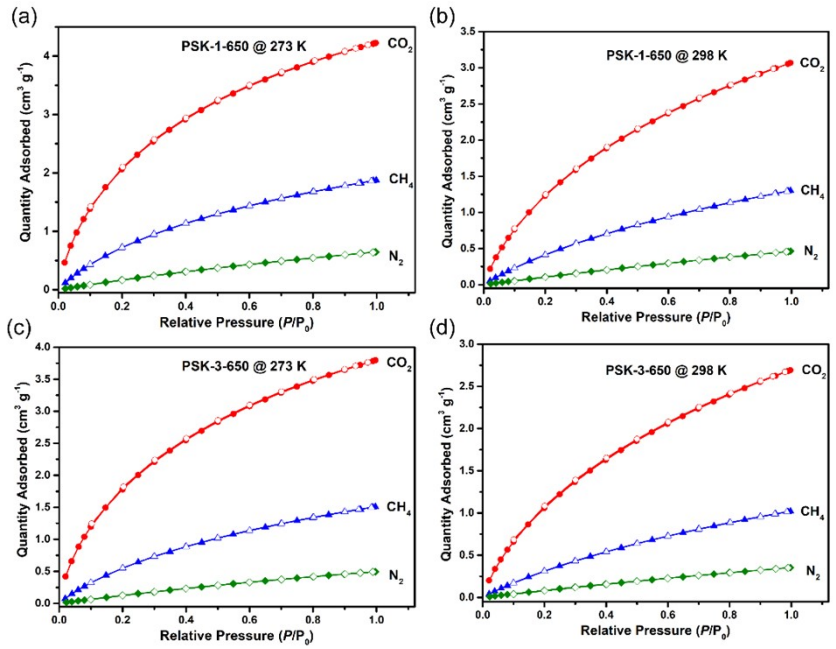

Figure S5. CO_2, CH_4, and N_2 adsorption-desorption isotherms of PS-derived carbons activated at 650 °C

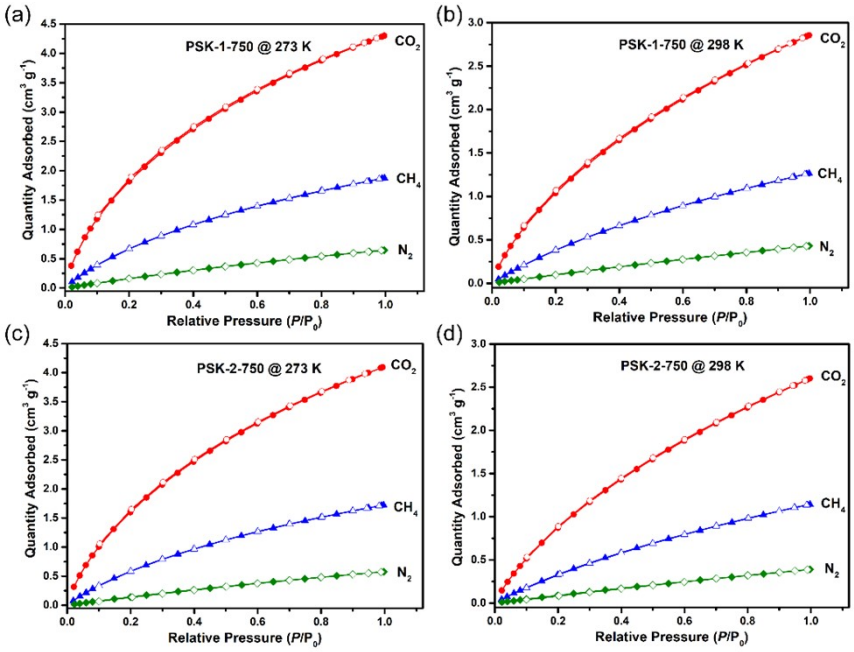

Figure S6. CO_2, CH_4 and N_2 adsorption-desorption isotherms of PS-derived carbons activated at 750 °C

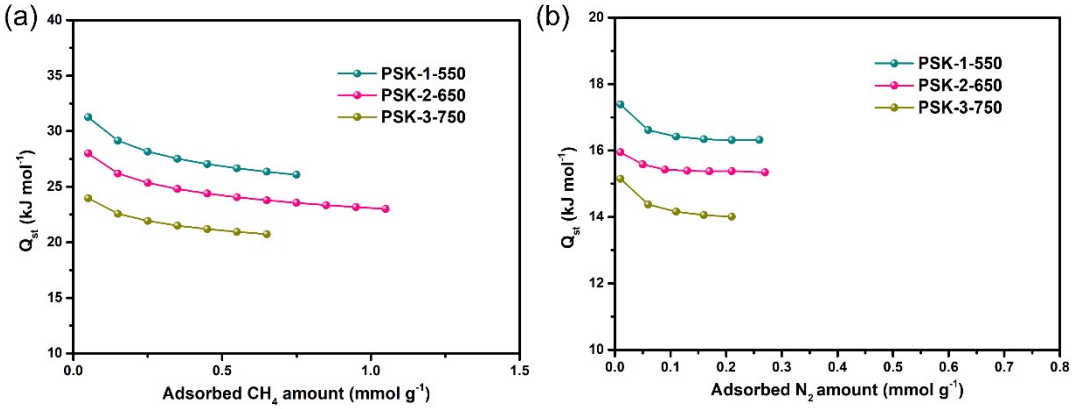

Figure S7. The figure of the isosteric adsorption heat on the CH_4; The figure of the isosteric adsorption heat on the N_2

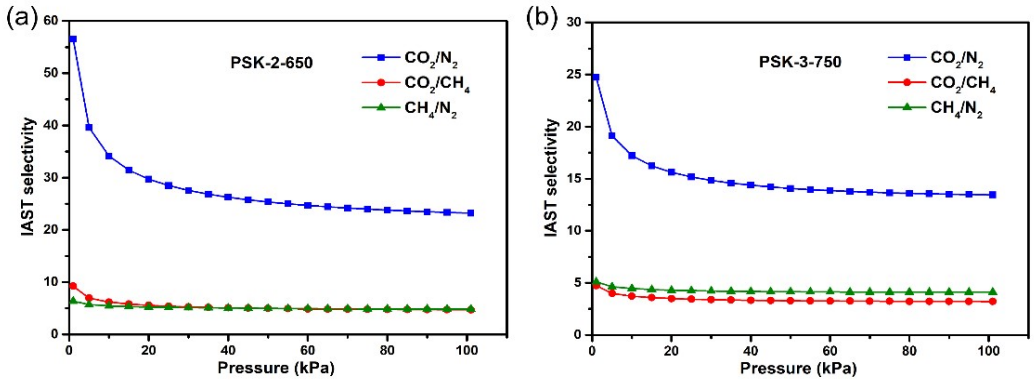

Figure S8. IAST selectivity of CO_2/N_2 (15:85), CO_2/CH_4 (10:90) and CH_4/N_2 (50:50) on (a) PSK-2-650 (b) and PSK-3-750 at 298 K.

Table S3. Comparison of adsorption properties of PS-derived carbons with other adsorbents.

Sample	CO_2 Uptake [a] (mmol g^{-1})	CO_2/N_2 [b] IAST Selectivity	Reference
PSK-1-550	2.70	32.7	This work
PSK-2-650	3.48	23.2	This work
PSK-3-750	2.21	13.5	This work
Arundo donax derived carbon	2.20	/	21
RLF-500	3.13	/	34
O-doped carbon adsorbents	3.46	26.5	35
phenolic resin	5.01	19	49
Bamboo-3-873	4.5	8.6	50
NPC-600	2.0	47.5	S3
azo-COP-1	1.5	63.7	S4

CS-500-1.5	2.7	23.1	S5
NC-1-500	1.4	63.0	33
R/HMTA-0.30	0.9	56.0	S6

[a] Measured at 298 K and 1 bar. [b] CO_2/ N_2 selectivity measured at 298 K and 1 bar.

Table S4. Comparison of adsorption and separation properties of PS-derived carbons with other adsorbents under 1bar.

Samples	CO_2 (mmol g^{-1}) 273 K	CO_2 (mmol g^{-1}) 298 K	CO_2/N_2 298 K	CO_2/CH_4 298 K	CH_4/N_2 298 K	Reference
OAC-1	5.41	3.46	26.5	4.5	4.6	35
OMC	3.0	2.0	12.8	3.4	3.7	51
Silicalite-1	-	2.00	-	2.6	3.5	52
TB-MOP	5.58	3.17	38.6	4	/	53
PF-600 KOH	/	3.23	41.7	6.8	/	54
PILCs	-	0.50	42	12.5	2.0	56
N-AC 600	6.36	4.3	47.3	9.2	3.6	57
PSK-1-550	3.35	2.70	32.7	7.1	4.6	This work
PSK-2-650	5.28	3.48	23.2	4.7	4.8	This work
PSK-3-750	4.11	2.21	13.5	3.2	4.1	This work

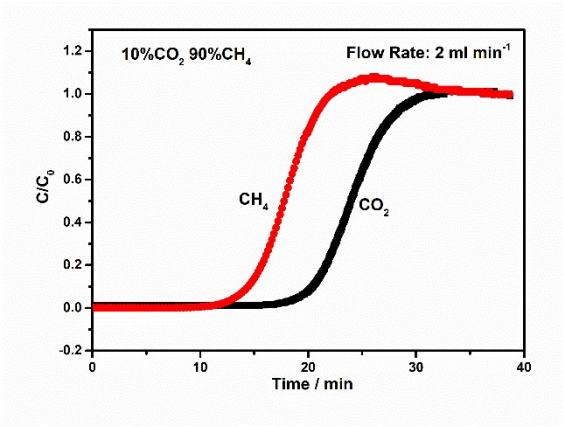

Figure S9. Breakthrough curves for PSK-2-650 at 298 K for CO_2/CH_4 (10:90) gas mixtures.

Reference

1 A. L. Myers, *Adsorption*, 2003, **9**, 9–16.

2 A. L. Myers and J. M. Prausnitz, *AIChE J.*, 1965, **11**, 121–127.

3 M. Lee, M. Park, H. Y. Kim and S. Park, *Nat. Publ. Gr.*, 2016, 1–11.

4 H. A. Patel, S. Hyun Je, J. Park, D. P. Chen, Y. Jung, C. T. Yavuz and A. Coskun, *Nat. Commun.*, 2013, **4**, 1357.

5 T. Chen, S. Deng, B. Wang, J. Huang, Y. Wang and G. Yu, *RSC Adv.*, 2015, **5**, 48323–48330.

6 F. Liu, K. Huang, Q. Wu and S. Dai, *Adv. Mater.,* 2017, **1700445**, 1–8.